Benzene, 1,4-dinitro-

Other names:	1,4-DINITROBENZOL, 1,4-Dinitrobenzene Benzene, p-dinitro- Dithane a-4 UN 1597 p-Dinitrobenzene para-Dinitrobenzene
Inchi:	InChI=1S/C6H4N2O4/c9-7(10)5-1-2-6(4-3-5)8(11)12/h1-4H
InchiKey:	FYFDQJRXFWGIBS-UHFFFAOYSA-N
Formula:	C6H4N2O4
SMILES:	O=[N+]([O-])c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	168.11
CAS:	100-25-4

Physical Properties

Property code	Value	Unit	Source
chs	-2894.00 ± 0.40	kJ/mol	NIST Webbook
chs	-2902.00	kJ/mol	NIST Webbook
ea	3.10 ± 0.05	eV	NIST Webbook
ea	2.00 ± 0.05	eV	NIST Webbook
ea	0.03	eV	NIST Webbook
ea	2.00 ± 0.10	eV	NIST Webbook
gf	173.52	kJ/mol	Joback Method
hf	36.37	kJ/mol	Joback Method
hfs	-38.00 ± 0.40	kJ/mol	NIST Webbook
hfus	27.67	kJ/mol	Joback Method
hsub	96.20 ± 2.50	kJ/mol	NIST Webbook
hsub	94.30 ± 0.70	kJ/mol	NIST Webbook
hvap	65.07	kJ/mol	Joback Method
ie	10.60 ± 0.10	eV	NIST Webbook
ie	10.50 ± 0.02	eV	NIST Webbook
ie	10.30 ± 0.10	eV	NIST Webbook
ie	10.65	eV	NIST Webbook
log10ws	-3.39		Aqueous Solubility Prediction Method
log10ws	-3.39		Estimated Solubility Method

logp	1.503		Crippen Method
mcvol	106.480	ml/mol	McGowan Method
pc	4730.11	kPa	Joback Method
rinpol	246.75		NIST Webbook
tb	672.02	K	Joback Method
tc	952.61	K	Joback Method
tf	446.70 ± 0.30	K	NIST Webbook
tf	446.65 ± 0.20	K	NIST Webbook
tf	444.20 ± 0.10	K	NIST Webbook
tf	446.82	K	Aqueous Solubility Prediction Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.63	J/mol×K	859.08	Joback Method
cpg	290.30	J/mol×K	905.85	Joback Method
cpg	254.14	J/mol×K	672.02	Joback Method
cpg	263.06	J/mol×K	718.79	Joback Method
cpg	271.07	J/mol×K	765.55	Joback Method
cpg	278.24	J/mol×K	812.32	Joback Method
cpg	295.30	J/mol×K	952.61	Joback Method
cps	200.00	J/mol×K	298.15	NIST Webbook
cps	192.00	J/mol×K	298.00	NIST Webbook
cps	167.00	J/mol×K	325.00	NIST Webbook
hfust	28.10	kJ/mol	446.65	NIST Webbook
hfust	28.12	kJ/mol	446.70	NIST Webbook
hfust	17.58	kJ/mol	446.00	NIST Webbook
hfust	28.12	kJ/mol	446.70	NIST Webbook
hfust	28.12	kJ/mol	446.70	NIST Webbook
hsubt	89.10 ± 1.70	kJ/mol	356.50	NIST Webbook
hsubt	89.00 ± 1.00	kJ/mol	343.00	NIST Webbook
hvapt	60.30	kJ/mol	508.50	NIST Webbook
psub	0.78	kPa	433.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range

psub	0.22	kPa	403.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	2.29e-04	kPa	323.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	1.66e-03	kPa	343.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	9.98e-03	kPa	363.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	0.06	kPa	383.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
sfust	62.90	J/mol×K	446.70	NIST Webbook
sfust	62.90	J/mol×K	446.65	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	456.20	K	4.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58941e+01
Coeff. B	-5.17139e+03
Coeff. C	-1.09129e+02
Temperature range (K), min.	440.49
Temperature range (K), max.	597.80

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.46557e+02
Coeff. B	-1.60028e+04
Coeff. C	-1.82393e+01
Coeff. D	5.60746e-06
Temperature range (K), min.	446.60
Temperature range (K), max.	803.00

Sources

Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range:	https://www.doi.org/10.1016/j.tca.2010.11.034
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100254&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1439
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1439

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume